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A posteriori error estimates for DDDAS inference problems

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Abstract

Inference problems in dynamically data-driven application systems use physical measurements along with a physical model to estimate the parameters or state of a physical system. Errors in measurements and uncertainties in the model lead to inaccurate inference results. This work develops a methodology to estimate the impact of various errors on the variational solution of a DDDAS inference problem. The methodology is based on models described by ordinary differential equations, and use first-order and second-order adjoint methodologies. Numerical experiments with the heat equation illustrate the use of the proposed error estimation machinery.

Keywords: Inverse problems, sensitivity analysis, DDDAS, data assimilation, a posteriori error

1 Introduction

Dynamically data-driven application systems (DDDAS [1]) is a paradigm whereby simulations and measurements become a symbiotic feedback control system. An important application of DDDAS is the solution of inference problems where information from physical measurements is combined with a mathematical model to obtain estimates of the state or parameters of a physical system. In practice both the data and the model are imperfect, and the corresponding errors directly impact the inference solution. This work discusses an a posteriori error estimation methodology to quantify the impact of data and model errors on specific aspects of the inference solution. A posteriori error estimates can give valuable insights about the stability and robustness of a DDDAS system. Our methodology is based on the variational framework and can have numerous applications in DDDAS. Examples include data assimilation, the dynamic steering of the measurement process to improve the overall forecasts [7], and dynamic location of faulty sensors.

A posteriori error estimation is a well established methodology in the context of finite element approximations of partial differential equations [4]. A posteriori error estimators for finite element methods in the solution of inverse problems are developed in [5, 6]. Related work has been done in the context of variational data assimilation problems to quantify the impact of

errors in the background, observations, and associated covariances [8, 9, 11]. Optimal solution error covariances for optimal control problems to estimate parameters, such as distributed model coefficients and boundary conditions for convection-diffusion model has been determined in [10].

While previous work has considered methodologies to estimate the impact of data errors, no method is available to date to estimate the impact of model errors on the optimal solution. Previously, the second order adjoint information has been used to solve PDE constrained optimization problems in [14]. This paper develops a coherent framework to estimate the impact of both model and data errors on the optimal solution. The computational procedure makes use of first order and the second order adjoint information and builds upon our previous work [16].

The paper is organized as follows. The DDDAS inference problem is introduced in Section 2. Section 3 describes the computational procedure for performing a posteriori error estimates. Numerical results in support of theoretical results are presented in Section 4. Concluding remarks are given in Section 5.

2 DDDAS inference

2.1 Fusing information from data and models

Data assimilation (DA) is the fusion of information from imperfect model predictions and noisy data, to obtain a consistent description of the state of a physical system [2, 3]. Two main approaches are in use for solving DA: variational and ensemble-based. The variational approach is based on optimal control theory, whereas the ensemble-based approach is rooted in statistical estimation theory. In this paper we focus on the variational approach. To obtain an estimate of the true state of a system \mathbf{x}^{true} three different sources of information are combined: the prior information, the model, and the observations. The best estimate that optimally fuses all these sources of information is called the analysis \mathbf{x}^{a} . The following subsections briefly describe the sources of information.

Prior information. The prior information encapsulates our current knowledge of the system. The prior information is captured by the background estimate of the state \mathbf{x}^{b} and the corresponding background error covariance matrix \mathbf{B} .

The model. The model captures our knowledge about the physical and chemical laws that govern the evolution of the system. The model evolves an initial state $\mathbf{x}_0 \in \mathbb{R}^n$ at the initial time t_0 to future states $\mathbf{x}_i \in \mathbb{R}^n$ at future times t_i . A general model equation is represented as follows:

$$\mathbf{x}_i = \mathcal{M}_{t_0 \rightarrow t_i}(\mathbf{x}_0) . \quad (1)$$

The observations. Observations represent the snapshots of reality available at discrete time instances. Specifically, measurements $\mathbf{y}_i \in \mathbb{R}^m$ of the physical state are taken at times t_i , $i = 1, \dots, N$

$$\mathbf{y}_i = \mathcal{H}^{\text{t}}(\mathbf{x}^{\text{true}}(t_i)) - \varepsilon_i^{\text{meas}}, \quad i = 1, \dots, N.$$

The observation operator \mathcal{H}^{t} maps the physical state space onto the observation space. The measurement errors are denoted by $\varepsilon_i^{\text{meas}}$.

The model state is related to observations by the following relation:

$$\begin{aligned} \mathbf{y}_i &= \mathcal{H}(\mathbf{x}_i) - \varepsilon_i^{\text{obs}}, \quad i = 1, \dots, N, \\ \varepsilon_i^{\text{obs}} &= \varepsilon_i^{\text{repres}} + \varepsilon_i^{\text{meas}}. \end{aligned} \quad (2)$$

The observation operator \mathcal{H} maps the model state space onto the observation space. The observation error term ($\varepsilon_i^{\text{obs}}$) accounts for both measurement and representativeness errors ($\varepsilon_i^{\text{repres}}$). The measurement errors can be attributed to faulty equipments. The representativeness errors are due to the inaccuracies of the numerical approximation inherent to the model.

2.2 Four dimensional variational data assimilation (4D-Var)

Variational methods solve the data assimilation problem in an optimal control framework. One finds the control variable which minimizes the mismatch between the model forecasts and the observations. In strong-constraint 4D-Var, the control parameters are the initial conditions \mathbf{x}_0 ; they uniquely determine the state of the system at all future times via the model equation (1). The background state is the prior knowledge of the initial conditions \mathbf{x}_0^b . Given the background value of the initial state \mathbf{x}_0^b , the covariance of the initial background errors \mathbf{B}_0 , the observations \mathbf{y}_i at t_i and the corresponding observation error covariances \mathbf{R}_i , $i = 1, \dots, N$, the 4D-Var problem provides the estimate \mathbf{x}_0^a of the true initial conditions by minimizing the following cost function:

$$\mathcal{J}(\mathbf{x}_0) = \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}_0^{-1} (\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2} \sum_{i=1}^N (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i), \quad (3)$$

subject to the constraint posed by the model equation (1).

In this paper, we consider a model (1) whose dynamics is described by a system of linear ordinary differential equations (ODEs)

$$\mathbf{x}' = \mathbf{A}\mathbf{x} + b(t), \quad t_0 \leq t \leq t_F, \quad \mathbf{x}(t_0) = \mathbf{x}_0 \quad (4)$$

where \mathbf{x}_0 , the vector of initial conditions, is not known accurately. The 4D-Var cost function in (3) can be rewritten in the integral form as follows:

$$\begin{aligned} \mathcal{J}(\mathbf{x}, \mathbf{x}_0) &= \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}_0^{-1} (\mathbf{x}_0 - \mathbf{x}_0^b) + \\ &\quad \frac{1}{2} \sum_{i=1}^N \int_{t_0}^{t_F} (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i) \delta(t - t_i) dt. \end{aligned} \quad (5)$$

The DDDAS inference problem of interest is formulated as follows:

$$\begin{aligned} \mathbf{x}_0^a &= \arg \min_{\mathbf{x}_0} \mathcal{J}(\mathbf{x}, \mathbf{x}_0) \\ &\text{subject to} \quad (4). \end{aligned} \quad (6)$$

The optimal solution for the inverse problem (6) can be found by using the adjoint sensitivity approach described extensively in [12] and [13].

We are interested in estimating the impact of observation and model errors on the inference result \mathbf{x}_0^a . Specifically, we will quantify the effect of errors on a certain aspect of the result. This quantity of interest is defined via a scalar error functional $\mathcal{E}(\mathbf{x}_0^a)$. In our case $\mathbf{x}_0^a \in \mathbb{R}^n$. One example of a quantity of interest on the k^{th} component of inference solution vector:

$$\mathcal{E}(\mathbf{x}_0^a) = (\mathbf{x}_0^a)_k, \quad (7)$$

Problem formulation. *We seek to quantify the impact that errors in the data and models used in DDDAS inference problems (6) have on a given aspect of the inference solution $\mathcal{E}(\mathbf{x}_0^a)$.*

2.3 The first order optimality conditions

The Lagrangian function associated with the cost function in (5) and the constraints in (4) is

$$\mathcal{L} = \mathcal{J}(\mathbf{x}, \mathbf{x}_0) - \int_{t_0}^{t_F} \lambda^T(t) \cdot (\mathbf{x}' - \mathbf{A}\mathbf{x} - b(t)) dt. \quad (8)$$

The optimality equations are obtained by setting the variations of the Lagrangian (8) to zero. The equation $\nabla_{\mathbf{x}}\mathcal{L} = 0$ leads to the following *adjoint ODE model*:

$$\lambda' = -\mathbf{A}^T \lambda - \mathcal{J}_{\mathbf{x}}, \quad \lambda(t_F) = 0, \quad (9a)$$

where

$$\mathcal{J}_{\mathbf{x}} = \sum_{i=1}^N \mathbf{H}_i^T \mathbf{R}_i^{-1} (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i) \cdot \delta(t - t_i),$$

and $\mathbf{H}_i = \mathcal{H}'(\mathbf{x}_i)$ is the linearized observation operator at \mathbf{x}_i .

Similarly, setting $\nabla_{\lambda}\mathcal{L} = 0$ we obtain the *forward ODE model* (4)

$$-\mathbf{x}' + \mathbf{A}\mathbf{x} + b(t) = 0, \quad \mathbf{x}(t_0) = \mathbf{x}_0. \quad (9b)$$

Furthermore, setting $\nabla_{\mathbf{x}_0}\mathcal{L} = 0$ we obtain the optimality equation

$$\mathbf{B}_0^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \lambda(t_0) = 0. \quad (9c)$$

Equations (9) constitute the first order optimality conditions for the inverse problem (6).

2.4 The super-Lagrangian

We follow the work done in [6, 16] to develop a posteriori error estimates which are applicable to our problem of interest. We first construct the Lagrangian associated with the error functional (24) and the constraints posed by the first order optimality conditions (9):

$$\begin{aligned} \mathcal{L}_{\mathcal{E}} = & \mathcal{E}(\mathbf{x}_0) - \int_{t_0}^{t_F} \mu^T \cdot (\lambda' + \mathcal{J}_{\mathbf{x}} + \mathbf{A}^T \lambda) dt - \mu^T(t_F) \cdot (\lambda(t_F) - 0) \\ & - \zeta^T \cdot (\mathbf{B}_0^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \lambda(t_0)) \\ & - \int_{t_0}^{t_F} \nu^T \cdot (-\mathbf{x}' + \mathbf{A}\mathbf{x} + b(t)) dt - \nu^T(t_0) \cdot (\mathbf{x}(t_0) - \mathbf{x}_0). \end{aligned} \quad (10)$$

Taking the variations of (10) and setting $\nabla_{\mathbf{x}_0}\mathcal{L}_{\mathcal{E}}$, $\nabla_{\lambda}\mathcal{L}_{\mathcal{E}}$, and $\nabla_{\mathbf{x}}\mathcal{L}_{\mathcal{E}}$ and to zero we obtain the following equations, respectively.

The Hessian equation

$$j_{\mathbf{x}_0, \mathbf{x}_0} \cdot \zeta = \left(\frac{d}{d\mathbf{x}_0^2} \mathcal{J}(\mathbf{x}(\mathbf{x}_0), \mathbf{x}_0) \right) \Big|_{\mathbf{x}_0^a} \cdot \zeta = \mathcal{E}_{\mathbf{x}_0} \quad (11)$$

can be solved using a quasi-Newton approximation of the reduced Hessian. This approximation is based on the sequence of reduced gradients obtained during the optimization. For additional details about the derivations, please refer to the extended version of this paper [15] .

The *tangent linear ODE model*

$$-\mu' + \mathbf{A} \cdot \mu = 0, \quad \mu(t_0) = \zeta(t_0) \quad (12)$$

is solved forward in time for the tangent linear variables μ .

Finally, the *second order adjoint ODE model*

$$\nu' = -\mathbf{A}^T \nu - \sum_i \mathbf{H}_i^T \mathbf{R}_i^{-1} (\mathbf{H}_i \cdot \mu_i) \cdot \delta(t - t_i) \quad (13)$$

is solved forward in time.

The procedure for computing the Lagrange multipliers for the super-Lagrangian (10) is summarized in Algorithm 1.

Algorithm 1 SuperLagrangeMultipliers

- 1: **procedure** SUPERLAGRANGEMULTIPLIERS
 - 2: Solve the reduced Hessian linear system (11) to obtain ζ .
 - 3: Solve the tangent linear model (12) to obtain μ .
 - 4: Solve the second order adjoint equation (13) to obtain ν .
 - 5: **end procedure**
-

3 A posteriori error estimation methodology

In practice, it is not possible for a model to completely represent the physics of reality. Consequently, the forward model (1) is inaccurate and subject to model errors. To describe this inaccuracy we consider a forward model (4) that is marred by a time dependent model error

$$\mathbf{x}' = \mathbf{A}\mathbf{x} + b(t) + \Delta b(t), \quad \mathbf{x}(t_0) = \mathbf{x}_0. \quad (14)$$

Moreover, the observation data \mathbf{y}_i in (2) is imperfect and marred by (additional) errors $\Delta\mathbf{y}_i$. This results in an error-marred cost function (3)

$$\begin{aligned} \hat{\mathcal{J}}(\mathbf{x}_0) &= \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}_0^{-1} (\mathbf{x}_0 - \mathbf{x}_0^b) \\ &\quad + \frac{1}{2} \sum_{i=1}^N (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i - \Delta\mathbf{y}_i)^T \mathbf{R}_i^{-1} (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i - \Delta\mathbf{y}_i) \\ &= \mathcal{J}(\mathbf{x}_0) + \Delta\mathcal{J}, \end{aligned} \quad (15)$$

where the error in the cost function is given by

$$\Delta\mathcal{J} = \sum_{i=1}^N -\Delta\mathbf{y}_i^T \mathbf{R}_i^{-1} (\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i) + \frac{1}{2} \Delta\mathbf{y}_i^T \mathbf{R}_i^{-1} \Delta\mathbf{y}_i. \quad (16)$$

In practice, instead of the ideal DDDAS inference problem (6) one solves the perturbed DDDAS inference

$$\begin{aligned} \hat{\mathbf{x}}_0^a = & \arg \min_{\mathbf{x}_0} \quad \hat{\mathcal{J}}(\mathbf{x}_0) \\ & \text{subject to} \quad (14). \end{aligned} \quad (17)$$

Our goal is to estimate the error in the optimal solution $\hat{\mathbf{x}}_0^a - \mathbf{x}_0^a$. Specifically, we seek to estimate the errors in the quantity of interest $\mathcal{E}(\mathbf{x}_0^a)$

$$\Delta \mathcal{E} = \mathcal{E}(\hat{\mathbf{x}}_0^a) - \mathcal{E}(\mathbf{x}_0^a).$$

The solution of the perturbed DDDAS inference (17) is subject to a perturbed set of optimality conditions (9). The error contributions to the optimal solution come from the errors in the adjoint model (9a), forward model (9b) and optimality equation (9c). This leads to the following change in error functional resulting from model and data errors

$$\Delta \mathcal{E} = \Delta \mathcal{E}_{\text{adj}} + \Delta \mathcal{E}_{\text{fwd}} + \Delta \mathcal{E}_{\text{opt}}. \quad (18)$$

From equation (10), the contribution to the error from the adjoint model is given by:

$$\Delta \mathcal{E}_{\text{adj}} = \sum_{i=1}^N \mu_i^T \cdot (\mathbf{R}_i^{-1} \mathbf{H}_i \Delta \mathbf{y}_i) \quad (19)$$

The contribution to the error brought by the forward model only depends on model errors:

$$\Delta \mathcal{E}_{\text{fwd}} = \int_{t_0}^{t_F} \nu^T \cdot \Delta b(t) dt. \quad (20)$$

The contribution to the error from the optimality equation can be computed from equation (10) as follows:

$$\Delta \mathcal{E}_{\text{opt}} = \zeta^T \cdot \left(\sum_{i=1}^N \left(\frac{\partial \mathbf{x}_i}{\partial \mathbf{x}_0} \right)^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \Delta \mathbf{y}_i \right). \quad (21)$$

Note that the quantity under the sum in (21) can be computed by *a single backward integration of the adjoint ODE model* (9a) using a forcing term

$$\mathcal{J}_{\mathbf{x}} = \sum_{i=1}^N \mathbf{H}_i^T \mathbf{R}_i^{-1} \Delta \mathbf{y}_i \cdot \delta(t - t_i).$$

The final formula for $\Delta \mathcal{E}$ can be obtained from (19), (20) and (21). The super-Lagrange multipliers required to perform the computations are obtained via Algorithm 1.

4 Numerical experiments

As a proof of concept we apply the error estimation algorithm to a test problem. The model is the one dimensional heat equation

$$\frac{\partial \mathbf{u}}{\partial t} = \alpha^2 \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2}, \quad \mathbf{x} \in [-1, 1], \quad t \in [0, 0.1] \quad (22)$$

	$\Delta\mathcal{E}_{\text{actual}}$	$\Delta\mathcal{E}_{\text{est}}$
Data Errors	1.945×10^{-2}	2.395×10^{-2}
Model Errors	2.561×10^{-2}	1.819×10^{-2}

Table 1: The comparison between actual error and the a posteriori error estimates for the heat equation.

with the following initial and boundary conditions:

$$\begin{cases} \mathbf{u}(0, \mathbf{x}) = u_0(\mathbf{x}), \\ \mathbf{u}(t, -1) = \mathbf{u}(t, 1), \\ \frac{\partial \mathbf{u}}{\partial \mathbf{x}}(t, -1) = \frac{\partial \mathbf{u}}{\partial \mathbf{x}}(t, 1). \end{cases} \quad (23)$$

We discretize the PDE (23) in space using a central difference scheme to obtain an ODE of the form (4), which is our forward model. The evolution of temperature with time is shown in the Figure 1(a). Synthetic observations are obtained by numerically integrating the forward model, started from the reference initial condition. Random observation errors are added to the values obtained by numerical integration. The observation errors are normally distributed with 0 mean and 10% standard deviation. Synthetic model errors are introduced by adding constants to the actual model; the imperfect model has the form (14) with $\Delta b(t) = 1$.

We solve the inverse problem (6) to obtain \mathbf{x}_0^a which minimizes the cost function (5). The quantity of interest, i.e., the error functional, is the mean value of the optimal initial condition

$$\mathcal{E}(\mathbf{x}_0^a) = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_0^a)_i. \quad (24)$$

The procedure outlined in Algorithm 1 and Section 3 is followed to estimate the impact of the data and model errors on the mean of the optimal solution (24). Solutions of the tangent linear, first order adjoint, and the second order adjoint models are shown in Figures 1(b), 1(c), and 1(d) respectively.

4.1 Results and discussion

We denote by \mathbf{x}_0^a the initial conditions obtained by solving the inverse problem (6), and by $\widehat{\mathbf{x}}_0^a$ the initial conditions obtained by solving the inverse problem (6). The actual error in the mean solution (24) is given by:

$$\Delta\mathcal{E}_{\text{actual}} = \mathcal{E}(\widehat{\mathbf{x}}_0^a) - \mathcal{E}(\mathbf{x}_0^a) = \frac{1}{n} \sum_{i=1}^n ((\widehat{\mathbf{x}}_0^a)_i - (\mathbf{x}_0^a)_i). \quad (25)$$

A posteriori estimates of this error $\Delta\mathcal{E}_{\text{est}}$ are calculated using the methodology discussed in Section 3. Table 1 compares the actual and the estimated errors in the mean initial values. We observe that the estimates are fairly accurate. Figure 2(a) shows the errors in the individual observations; they are randomly distributed. Figure 2(b) shows the contributions of different observation errors to the error in the quantity of interest (24). We observe that certain grid points contribute to the error more than others. Since the physical process is diffusive, measurements errors occurring earlier in time contribute more to the a posteriori error estimate. The data error contributions indicate the sensitive areas, where measurements need to be very

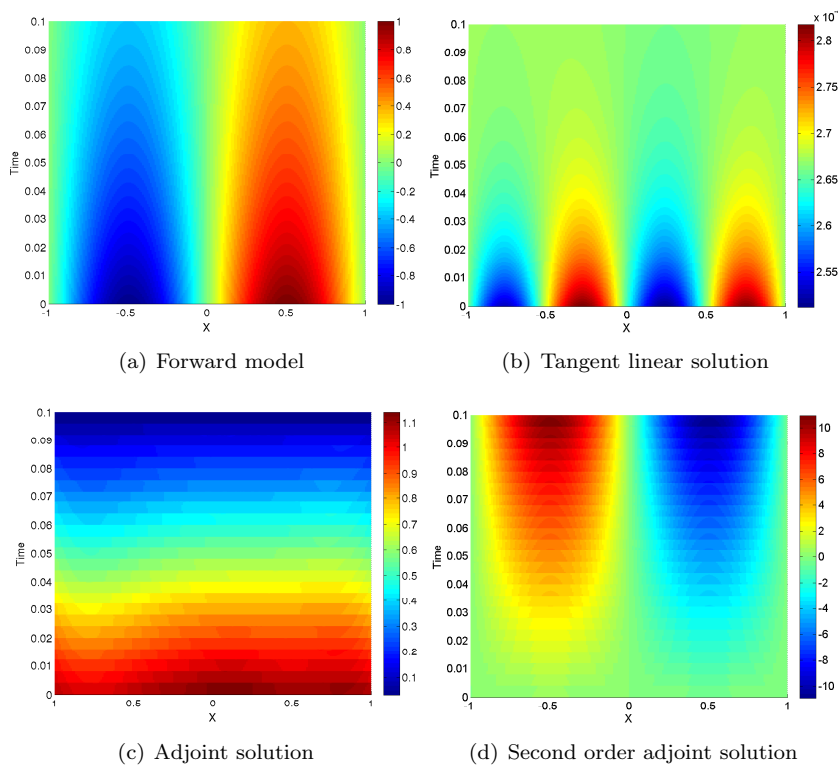


Figure 1: The evolution of forward, tangent linear, and adjoint variables for the heat equation.

accurate. Gross inconsistencies in the data error contribution may also point towards faulty sensors. Figure 2(c) shows the contributions of model errors at different grid points to the error in the quantity of interest (24). We observe that the contributions of model errors follows the profile of the second order adjoint model evolution shown in Figure 1(d). This is in agreement with the theory in Section 2. Some grid points tend to be more sensitive than the others to the errors in the model. This indicates the need for better physical representation, e.g., obtained by increasing grid resolution in the sensitive regions.

5 Conclusions

DDDAS inference problems are solved in practice using imperfect models and imperfect data. The errors in the model and data impact the result of the inference. This work develops a methodology to estimate the impact of model and data errors on the inference result. The a posteriori error estimation is applied after solving the inverse problem. The approach considers a scalar quantity of interest that depends on the inference result, and that is formalized as an error functional. The errors in the quantity of interest due to errors in the model and data are estimated to first order using an algorithm that involves tangent linear, first, and second order adjoint models. While the presentation here uses linear ODE models the theoretical framework can be extended to any inverse problem. We illustrate the proposed approach using a data assimilation test for the one dimensional heat equation. For this example the error estimates

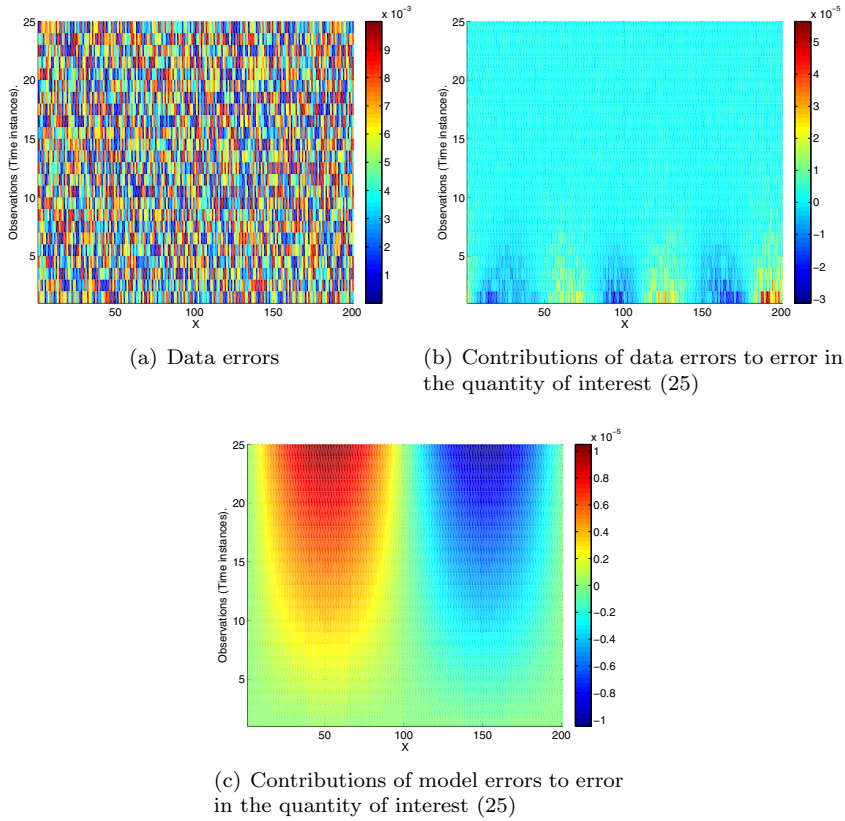


Figure 2: Data errors at different grid points and the contributions to the error functional resulting from data and model errors.

are very close to the actual errors in the quantity of interest due to both the data as well as the model inaccuracies.

The proposed methodology can prove useful in a general DDDAS context to quantify and reduce uncertainties in the system. The error estimates can be used to locate faulty observations. Moreover, the areas of maximum sensitivity highlighted via the error estimates indicate the locations where greater accuracy in measurements is required (adaptive observations), or where it is beneficial to increase the model resolution (adaptive modeling).

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